The virial equation of state for unitary fermion thermodynamics with non-Gaussian correlations

Ji-sheng Chen*,   Jia-rong Li,   Yan-ping Wang,   and   Xiang-jun Xia

Physics Department & Institute of Particle Physics,
Central China Normal University, Wuhan 430079, People's Republic of China

(Dated: December 15, 2008)

We study the roles of the dynamical high order perturbation and statistically non-linear infrared fluctuation/correlation in the virial equation of state for the Fermi gas in the unitary limit. Incorporating the quantum level crossing rearrangement effects, the spontaneously generated entropy departing from the mean-field theory formalism leads to concise thermodynamical expressions. The dimensionless virial coefficients with complex non-local correlations are calculated up to the fourth order for the first time. The virial coefficients of unitary Fermi gas are found to be proportional to those of the ideal quantum gas with integer ratios through a general term formula. Counterintuitively, contrary to those of the ideal bosons ($a_2^{(0)} = -\frac{1}{4\sqrt{2}}$) or fermions ($a_2^{(0)} = \frac{1}{4\sqrt{2}}$), the second virial coefficient a_2 of Fermi gas at unitarity is found to be equal to zero. With the vanishing leading order quantum correction, the BCS-BEC crossover thermodynamics manifests the famous pure classical Boyle's law in the Boltzmann regime. The non-Gaussian correlation phenomena can be validated by studying the Joule-Thomson effect.

I. INTRODUCTION

Unconventional unitary fermion physics is associated with a variety of strongly interacting topics. This theme can test the many-body theories, from neutron stars and nuclear matter to quark-gluon plasmas etc.

In recent years, the study for the interacting fermion matter properties has attracted much attention in quantum many-body community[1]. This is attributed to the rapid progress of atomic Fermi gas experiments. Controlling the S-wave scattering length between two different spin components allows one to control the interaction strength by using a magnetically tuned Feshbach resonance. With the magnetic tuning technique, increasing the interaction strength of atomic fermions with scattering length a from $-\infty$ to $+\infty$ resulting in bound boson systems exhibits the Bardeen-Cooper-Schrieffer to Bose-Einstein condensation (BCS-BEC crossover). The two regimes with positive and negative S-wave scattering length meet in the strongly interacting limit with the divergent scattering length. At the resonant point, the scattering cross-section will be saturated as $\sigma = 4\pi/k^2$ (with k being the relative wave-vector magnitude of the colliding particles) due to the fundamental unitary property limit. The strongly interacting BCS-BEC crossover topic is literally called the unitary Fermi gas thermodynamics[1–16].

Generally, the thermodynamical properties of the low energy dilute Fermi system are determined by the S-wave scattering length a, the particle number density n as well as the temperature T. In the resonant regime

with a zero-energy bound state, the divergent scattering length will certainly drop out in the thermodynamical quantities; i.e., the thermodynamical properties are universal[1–3]. The divergent scattering length poses an intractable many-body problem.

In addressing the BCS-BEC crossover thermodynamics, the fundamental issue is the ground state energy. On the basis of the dimensional analysis, the dimensionless coefficient ξ relates the energy per particle $E/N = \xi\frac{3}{5}\epsilon_f$ with the Fermi kinetic energy $\epsilon_f = k_f^2/(2m)$. Here, m is the bare fermion mass while k_f is the Fermi momentum. The fundamental universal coefficient ξ has prompted many theoretical or experimental efforts in recent years[1]. Furthermore, the finite temperature thermodynamic properties of unitary Fermi gas are as intriguing as the zero-temperature ground state energy and many experimental/theoretical efforts have been made[5, 6][7, 8].

Compared with the zero-temperature ground state energy, the additional energy scale, i.e, the reciprocal thermodynamical de Broglie wavelength $\lambda^{-1} = \sqrt{mT/(2\pi)}$ complicates the theme and makes the universal property analysis more profound[3]. In the weak degenerate Boltzmann regime, the universal properties are characterized by the virial coefficients [3, 4, 9, 15]. For example, the virial equation of state is related with the neutrinosphere physics in supernovae for the dilute nuclear matter matter. It is believed that the virial equation of state will influence the detailed information of the neutrino response of low-density neutron matter[9]. How to calculate the virial coefficient in the unitary limit regime remains an important many-body topic. Like in addressing the zero-temperature ground state energy problem, the central task is to understand the novel non-linear fluctuation/correlation physics.

*chenjs@iopp.ccnu.edu.cn

The virial expansion is the basic tool for use in discussing the thermodynamical properties and should be model independent. In thermodynamics, the non-linear virial expansion is the *infinite* series of the pressure according to the particle number density. Even as a fundamental theme, this question is very challenging and by no means resolved yet. To derive the high order virial coefficients of strongly correlated fermions in the unitary limit, the involved quantum statistical fluctuation/correlation and detailed dynamical effects must be clarified, which is the novel systematic requirement for the sound theoretical efforts. With the aim of calibrating the universal virial coefficients, we strive to examine the spontaneously quantum level shift contribution on the entropy (counting the microscopic states) in a dynamically and thermodynamically self-consistent way.

In this work, the dynamical and statistical correlation analysis explicitly demonstrates that the dense and hot thermodynamics at unitarity obey the virial theorem for the ideal non-interacting gas, i.e., $P = 2/3E/V$[3, 5]. Meanwhile, the calculated virial coefficients at unitarity are found to be proportional to those for the ideal Fermi gas with integer ratios through an universal *general term formula*.

In the strongly interacting system, the dynamical effects compete with the non-linear fluctuation/correlations. The second virial coefficient is found to be vanishing due to the complicated correlations. From the viewpoint of bulk properties, is the dilute unitary Fermi gas behavior much more like the classical ideal Boyle gas in the weak degenerate Boltzmann regime?

The present paper is organized as follows. In Sec.II, the statistical method with effective field theory formalism is presented. The approach is promoted by the phase separation-instability discussions for a compact environment containing a competitive Coulomb frustration element. In this work, we will take into account the novel non-Gaussian fluctuation effects on the strongly interacting fermions thermodynamics. The thermodynamical consistency, virial theorem discussion and the high order virial coefficient calculations of the unitary Fermi system are presented in Sec.III. The numerical results are also presented in this section in order to allow comparison with previous investigations. In Sec.IV, the scaling property of equation of state and the virial expansion in the unitary regime are further analyzed. Summarizing remarks are made in Sec.V.

The calculations are performed in terms of the universal four-fermions contact interaction formalism. The natural units $k_B = \hbar = 1$ are used throughout the paper.

II. STATISTICAL DYNAMICS WITH NON-GAUSSIAN CORRELATIONS

The strongly interacting matter offers a plausible perspective in looking for the general statistical field theory methods. In the presence of a medium, the unitary topic becomes very challenging because the system is strongly correlated and has no small parameter applicable for any controlled perturbative calculations.

Essentially, the strong correlation effects are highly non-linear and the pronounced turbulent features will appear in the unitary system. The conventional mean-field theory or loop diagram ring and ladder resummation perturbative techniques cannot be employed for the unitary fermions. Consequently, more theoretical attempts are urgently needed to understand the detailed dynamical role of the strongly interacting fermions thermodynamics. Although there are tremendous updating efforts, a soundly exact theory concerning the behavior at unitarity is still not available.

With the goal of calculating the high order virial coefficients, the procedure developed can allow the systematic rearrangements of the individual expansions while avoiding the theoretical double countings. The thermodynamical expressions obtained are in parallel with those with the linear bare contact interaction formalism. Therefore, the method developed will be referred to as the *quasi-Gaussian/quasi-linear approximation* in order to indicate the difference from and similarity to lowest order mean-field theory.

A. In-medium effective action

The in-medium behavior associated with the many-body characteristic is the key, while a non-perturbative approach is crucial. In many-body theory, an established fundamental perspective is that particles can change their spectrum properties in a dense and hot strongly correlated medium. These changes will be reflected in the mass shifts and/or in the development of excited complex spectral property modifications. Considering the counteracting influences of the surrounding medium and spontaneous single-particle spectrum modification due to the off-shell dispersive effects, a medium-scaling functional has been proposed[17]

$$
\begin{aligned}
\tilde{H} = &- \int d^3x \psi_\alpha^*(x)(\frac{\nabla^2}{2m} - \mu_{r\alpha}[n, T])\psi_\alpha(x) \\
&+ \frac{U_{\text{eff}}^*[n, T]}{2} \int d^3x \psi_\alpha^*(x)\psi_\beta^*(x)\psi_\beta(x)\psi_\alpha(x).
\end{aligned} \quad (1)
$$

In Eq.(1), $\alpha, \beta = \uparrow, \downarrow$ represent the (hyperfine-)spin projection Ising-variable. The effective Hamiltonian is the same as the original Bethe-Peierls zero-range contact interaction version, except that the bare coupling constant $U_0 = 4\pi a/m$ is substituted by an effective medium-scaling functional $U_{\text{eff}}^*[n, T]$. With the bare potential U_0 and corresponding vanishing $\mu_{r\alpha}$ in the vacuum limit $n \to 0$, the Hamiltonian $\tilde{H}$ reduces to the original version possessing a global $U(1)$ or Z_2 gauge symmetry.

Due to the explicit medium dependence of U_{eff}^* in Eq.(1), we introduce the additional counterterm $\delta\mathcal{H} \propto$

$\mu_r[n,T]$, which is enforced by the fundamental thermodynamical Hugenholtz-van Hove (HvH) theorem[18, 19]. Without loss of generality, we take care of the fully symmetric scenario with $\mu_{r\alpha} = \mu_r$. The complementary $\delta\mathcal{H}$ implies that the correlation effects on the single particle energy spectrum are further taken into account as an effective single-body potential or spontaneously generated binding energy in the spirit of density functional theory[20]. On average, the thermodynamic vacuum will have been "shifted" by $\mu_r N$ non-perturbatively.

As remarked in Ref.[17, 21], the central ingredient of this non-perturbative procedure is the way of deriving the correlating coupling functional U_{eff}^*. Essentially, its constitution is beyond the bare Bethe-Peierls dynamics itself; i.e, the derivation of U_{eff}^* must be based on a more underlying physical law[18]. The functional U_{eff}^* should reasonably encode the non-perturbative counteracting effects of the surrounding environment.

In thermodynamics, the surrounding environment plays a counteracting frustration role according to Le Chatelier's stability principle. This general principle accounts for the environment preventing an instantaneous departure from equilibrium with an alternating minus function[17, 22], which is consistent with the second law of thermodynamics. We find that the frustrating correlation effects of the surrounding environment can be realized via a twisted composite rearrangement matrix-vertex[17]

$$U_{\text{eff}}^* = \frac{U_0}{1 - (m_D^2/2)U_0}, \qquad (2)$$

$$\downarrow$$

$$a_{\text{eff}} = \frac{a}{1 - (2\pi m_D^2/m)a}. \qquad (3)$$

In order to making the analytical expressions as concise as possible, the inverse scattering length notation employed, a_{eff}, is defined in terms of $U_{\text{eff}}^* \equiv 4\pi a_{\text{eff}}/m$.

The reader will have noticed that there is an alternating "negative" sign difference in the denominator of Eq.(2) compared with the loop ring and ladder resummation perturbative techniques; i.e., the medium-scaling potential Eq.(2) appears as an instantaneously anti-screening formalism. This specific minus sign leads to quite different physical motivations and calculational details. The non-linear screening formalism makes it possible for us to incorporate the intermediate off-shell effects in an analytical way with 4-momentum independent algebra equations, i.e., instead of numerically solving the various coupled integral equations for the multi-points correlation Green functions. This refreshing attempt is motivated by the particular conformal analogy and/or discursion of the zero-range unitary Fermi problem with the universal instantaneous Coulomb correlation discussions in a compact confinement environment[23, 24] based on the relativistic continuum Dirac field theory formalism [25, 26], where involves the complex oscillatory instabilities with short range and long-range force's competitions.

By analogy to the generalized Dyson-Schwinger calculations with finite temperature Green function theory[17, 21], but more conveniently, the Debye mass parameter m_D^2 in Eq.(2) can be alternatively given by the generalized Ward-Identity

$$m_D^2 = \left(\frac{\partial n}{\partial \mu^*}\right)_T = \frac{2}{T\lambda^3} f_{1/2}(z') \equiv 2\chi', \qquad (4)$$

where μ^* is the effective chemical potential, the collective implicit variable defined below. At $T = 0$, it reduces to the familiar $m_D^2 = k_f m/\pi^2 = 2N(\epsilon_f)$, where $N(\epsilon_f)$ is the unperturbated density of states on the Fermi surface for one component fermions[27]. m_D^2 characterizes the fluctuation physics because it is related to the well-known Pauli paramagnetic spin-spin or particle number susceptibility $\chi = \frac{1}{2}(\partial n/\partial\mu)_T$ (with an additional factor $\frac{1}{2}$ due to the degenerate degrees of freedom of the two-components symmetric system) according to

$$(\partial n/\partial\mu)_T = (\partial n/\partial\mu^*)_T\,(\partial\mu^*/\partial\mu)_T. \qquad (5)$$

B. Grand thermodynamical potential with quasi-Gaussian approximation

From the general Lagrange multiplier viewpoint, what we will perform is an evaluation of the relative minimum $\tilde{\Omega}(T, \tilde{\mu})$ of the shifted $\langle\tilde{0}|H - (\mu - \mu_r)N|\tilde{0}\rangle$ instead of directly evaluating the challenging absolute minimum $\Omega(T, \mu)$ of the grand thermodynamic potential $\langle 0|H - \mu N|0\rangle$[17, 21]. With auxiliary physical constraints, the realistic $\Omega(T, \mu)$ incorporating the thermodynamical vacuum fluctuation and correlation effects is indirectly derived from the former for the given chemical potential μ.

Firstly, the shifted relative minimum is evaluated by freezing the medium-dependent interaction potential with the conventional condensation formalism[17, 21]

$$\frac{\tilde{\Omega}(T, \mu^*)}{V} = -P + \mu_r n$$
$$= -\frac{\pi a_{\text{eff}}}{m}n^2 - 2T\int_k \ln(1 + e^{-\beta(\frac{\mathbf{k}^2}{2m} - \mu^*)}), (6)$$

with $\int_k = \int d^3\mathbf{k}/(2\pi)^3$ being the momentum integral. The constraining self-consistent equation for the single particle Green function gives the definition of the effective chemical potential μ^* according to

$$\tilde{\mu} = \mu - \mu_r = \frac{2\pi a_{\text{eff}}}{m}n + \mu^*. \qquad (7)$$

The total number density $n = n_\uparrow + n_\downarrow = 2n_\uparrow$ is given by

$$2\int_k f_k \equiv n(T, \mu^*), \qquad (8)$$

with the defined quasi-particle Fermi-Dirac distribution functions

$$f_k = \frac{1}{z'^{-1}e^{\beta\frac{\mathbf{k}^2}{2m}} + 1}, \quad z' = e^{\beta\mu^*}. \qquad (9)$$

Different from the multiplier chemical potential μ, the dynamically collective variable μ^* characterizes the additional correlation effects. With the chemical potential correction, the *effective fugacity* z' is analogous to the conventional one $z = e^{\beta\mu}$. Employing the quasi-particle Fermi-Dirac distribution functions Eq.(9), the thermodynamical formulae can manifest the standard Fermi integrals $f_j(z')$ with $j = -\frac{1}{2}, \frac{1}{2}, \cdots$.

Secondly, the remaining task is to determine the correction term with physical constraints, from which the realistic grand thermodynamical potential will be uniquely determined. The shift terms $\propto \mu_r$ in the pressure and chemical potential are canceled out by each other in the Helmholtz free energy density $f = F/V = -P + \mu n$. However, the analytical expression for the relative shift strength μ_r can be indirectly derived from the physical free energy density by relaxing the *medium dependence* of interaction potential.

Invoking the thermodynamical relations, one can have

$$P = n^2 \left(\frac{\partial (f/n)}{\partial n} \right)_T, \qquad (10)$$

$$\mu = \left(\frac{\partial f}{\partial n} \right)_T. \qquad (11)$$

Comparing the results derived from Eq.(10) and Eq.(11) with Eq.(6) or Eq.(7), one has the definite analytical expression of the relative shift strength

$$\mu_r[n, T] = \mathcal{C}(T, \mu^*) \left(\frac{2\pi a_{\text{eff}}}{m} \right)^2 n^2. \qquad (12)$$

The employed correlation factor $\mathcal{C}$ is defined by

$$\mathcal{C}(T, \mu^*) \equiv m_D \left(\frac{\partial m_D}{\partial n} \right)_T = \frac{f_{-1/2}[z']}{2T f_{1/2}[z']}. \qquad (13)$$

m_D^2 and $\mathcal{C}(T, \mu^*)$ are related to the high order density/spin susceptibilities; i.e., they have the crystal clear physical connotations. With these two physical variables, the integrated grand partition function Eq.(6) or scaling equation of state and chemical potential Eq.(7) are reduced to

$$P = P_{\text{ideal}}(T, \mu^*) + \frac{\pi a_{\text{eff}}}{m} n^2 + \mathcal{C} \left(\frac{2\pi a_{\text{eff}}}{m} \right)^2 n^3 \quad (14a)$$

$$\mu = \mu^* + \frac{2\pi a_{\text{eff}}}{m} n + \mathcal{C} \left(\frac{2\pi a_{\text{eff}}}{m} \right)^2 n^2, \qquad (14b)$$

with

$$P_{\text{ideal}} \equiv \frac{2T}{\lambda^3} f_{5/2}(z'), \qquad (15)$$

which is similar to the ideal Fermi gas but with the effective chemical potential as the collective variable.

In Eq.(14a) and Eq.(14b), the first two terms appear as those obtained with the canonical Gaussian integral

formalism via the frozen interaction; i.e., they have exactly the same structure of mean-field theory with linear-like interaction. The last curious shift term in Eq.(14a) non-Gaussianly proportional to the cubic particle number density, $\propto n^3$, characterizes the high order contributions beyond the former. This spontaneously generated term is picked up in a thermodynamical way by resuming the medium dependence of the interaction matrix. Physically, this rearrangement effect considerably shifts the chemical potential of the particle distribution function as displayed by Eq.(14b).

The correlation contributions manifested by the factor $\mathcal{C}$ are explicitly combined with the dynamical high order ones.

It is of crucial importance that the low and high order contributions are mixed with each other through a collective variable, μ^*, effective chemical potential. One can see that the grand thermodynamical potential $\Omega(T, \mu)$ is not the naive polynomial expanded according to the bare vacuum interaction strength U_0. The dependence of the grand thermodynamical potential Ω on the collective correlation variable μ^* can be numerically eliminated in favor of the realistic physical chemical potential μ. It is physically pretty satisfactory that the equations Eq.(14a) and Eq.(14b) include the highly non-linear or turbulent correlation contributions. In the weak coupling limit, the equations readily reduce to those in terms of the lowest order mean-field theory, where the non-linear fluctuation/correlation contributions disappear.

III. THERMODYNAMICS WITH QUANTUM REARRANGING CORRELATIONS

We now examine the thermodynamical quantities with the self-consistent equations or the grand partition function Eq.(14a) with Eq.(14b). The scenario we present is quite general although we have restricted ourselves to the low energy long-wavelength thermodynamics of the ideal fully symmetric system. For instance, the formalism and expressions can be easily extended to the asymmetric fermions phase separation analysis with unequal populations[28].

A. Thermodynamical consistencies, entropy and energy densities

As discussed above, the non-Gaussian correlation effects considerably complicate the one-one Legendre corresponding relation of particle number N and the multiplier chemical potential μ in the strongly interacting systems. Due to the explicit high order corrections for the physical chemical potential, the calculations require additional great care; i.e., one must check if the thermodynamical relations are exactly ensured before making further discussions.

For instance, an obvious check is to verify that the

partial derivative of P according to μ gives again the particle number density $n = N/V$ Eq.(8)

$$n = \left(\frac{\partial P}{\partial \mu}\right)_T = \left(\frac{\partial P}{\partial \mu^*}\right)_T \left(\frac{\partial \mu^*}{\partial \mu}\right)_T = \frac{2}{\lambda^3} f_{3/2}(z'). \quad (16)$$

Eq.(16) is one of the stringent thermodynamic conditions which are automatically satisfied by our nonperturbative approach. Therefore, the grand partition function Eq.(14a) can give the exact virial coefficients.

Furthermore, the energy density and heat capacity can be given by the dimensionless virial coefficients in the dilute Boltzmann regime. This provides a novel requirement for the effective field theory. The complication of the temperature dependent interaction provides additional task to check the thermodynamic consistency characterized by the one-one Legendre correspondence relation between T and entropy S.

According to the thermodynamical relations for $s = S/V$ and $\epsilon = E/V$

$$s = \left(\frac{\partial P}{\partial T}\right)_\mu, \quad (17a)$$

$$\epsilon = -T^2 \frac{\partial}{\partial T}\left(\frac{-P + \mu n}{T}\right)_n, \quad (17b)$$

and using partial derivative formulae such as

$$\left(\frac{\partial \mu^*}{\partial T}\right)_\mu \left(\frac{\partial T}{\partial \mu}\right)_{\mu^*} \left(\frac{\partial \mu}{\partial \mu^*}\right)_T = -1, \quad (18a)$$

$$\left(\frac{\partial m_D^2}{\partial T}\right)_n = \left(\frac{\partial m_D^2}{\partial T}\right)_{\mu^*} + \left(\frac{\partial m_D^2}{\partial \mu^*}\right)_T \left(\frac{\partial \mu^*}{\partial T}\right)_n \quad (18b)$$

the integrated entropy and energy densities read

$$s = s_{\text{ideal}} + \mathcal{D}\left(\frac{2\pi a_{\text{eff}}}{m}\right)^2 n^2, \quad (19a)$$

$$\epsilon = 2\int_k \frac{k^2}{2m} f_k + \frac{\pi a_{\text{eff}}}{m} n^2 + T\mathcal{D}\left(\frac{2\pi a_{\text{eff}}}{m}\right)^2 n^2 \quad (19b)$$

In the above equations, we have employed the notation

$$s_{\text{ideal}} \equiv -2\int_k \left[f_k \ln f_k + (1 - f_k)\ln(1 - f_k)\right], \quad (20)$$

with that for the correlation factor

$$\mathcal{D}(T, \mu^*) = \frac{\left(\frac{\partial^2 n}{\partial \mu^{*2}}\right)_T \left(\frac{\partial n}{\partial T}\right)_{\mu^*} - \frac{\partial^2 n}{\partial T \partial \mu^*}\left(\frac{\partial n}{\partial \mu^*}\right)_T}{2\left(\frac{\partial n}{\partial \mu^*}\right)_T}. \quad (21)$$

The first term in entropy density Eq.(19a) and first two terms in energy density Eq.(19b) constitute the conformal formalism of ideal Fermi gas or mean-field theory but with the effective chemical potential. Significantly, there is an additional (last) spontaneously generated term $\propto \mathcal{D}(T, \mu^*)$ resulting from the quantum level rearrangement. These extra terms are the explicit dynamical high

order contributions and of non-Gaussian characteristic. As explicitly indicated by Eq.(21), the high order effects are mixed with the fluctuations through the temperature and particle number density susceptibilities. These contributions are vanishing in the zero-temperature conditions. Therefore, they do not affect the previous zero-temperature universality property discussions[17, 21, 23]. Furthermore, they are canceled out by each other exactly in the physical Helmholtz free energy density $f = \epsilon - Ts$ and consequently can be easily neglected. The present recipe rectifies the drawback.

With the analytical expressions, we have indicated the entropy per particle versus the rescaled energy in Fig.1. One can see that although the high order contributions can be almost neglected in the low temperature regime, they play a significant role with the increase of temperature (energy density). In comparison to that for the mean-field theory without the non-Gaussian correlation contribution, the convex behavior of the entropy curve more closely approaches the experimental result or numerical simulations[6]. For comparison, we have also given the curve for the ideal free Fermi gas.
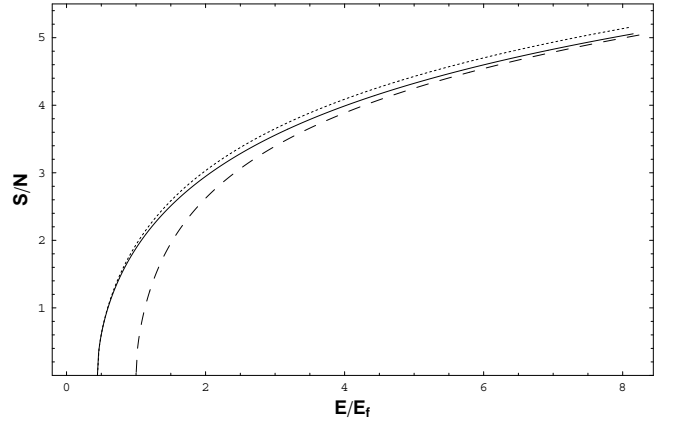

FIG. 1: Entropy per particle versus rescaled energy at unitarity[6]. The solid curve is for the theoretical value including the spontaneously generated contribution while the dotted one is for the mean-field theory result. The below dashed curve is that for the free Fermi gas.

B. Virial theorem and universal coefficient $\xi(T)$ at finite temperature

In order to justify the validity of our quasi-Gaussian approximation, the virial theorem for the dense and hot unitary Fermi gas will be strictly re-examined and proved.

The non-Gaussian correction terms appear in the pressure and energy density, simultaneously. At unitarity, the general analytical expressions for the pressure, Eq.(14a)

and energy density, Eq.(19b), are reduced to

$$\epsilon = \frac{3T}{\lambda^3}\left(f_{5/2}(z') - \frac{f_{3/2}^2(z')}{2f_{1/2}(z')} + \frac{f_{3/2}^3(z')f_{-1/2}(z')}{2f_{1/2}^3(z')}\right)$$
$$= \frac{3}{2}P. \tag{22}$$

Eq.(22) explicitly demonstrates that the unitary Fermi gas thermodynamics obeys the virial theorem of ideal gas[3, 5]. What we want to emphasize is that the crucial high order non-Gaussian fluctuation terms ensure the virial theorem and the zero-temperature HvH theorem.

The energy density manifests the scaling property as displayed by Eq.(22). The universal coefficient $\xi(T)$, i.e, the ratio of the unitary Fermi gas energy density to that of the ideal ones, can be given as a function of z'

$$\xi(T) = 1 - \frac{f_{3/2}^2(z')}{2f_{1/2}(z')f_{5/2}(z')} + \frac{f_{3/2}^3(z')f_{-1/2}(z')}{2f_{1/2}^3(z')f_{5/2}(z')}. \tag{23}$$

The effective fugacity z' is uniquely determined by the particle number density according to Eq.(8) or Eq.(16) for fixed temperature T.

As shown in Fig.2, the universal coefficient approaches the expected saturation value $\xi = 1$ in the Boltzmann limit. It is worthy noting that in the low temperature strong degenerate regime with $T_f/T \gg 1$, the effective fugacity can be explicitly indicated as $z' = e^{T_f/T}$, where T_f is Fermi characteristic temperature. As stressed in [17, 21], the zero-temperature result $\xi(0) = \frac{4}{9}$ is consistent with the existing theoretical calculations [10, 12] and experimental measurements[6, 32, 33].

In Fig.3, we have presented the finite temperature thermodynamical numerical results. They are reasonably consistent with previous theoretical investigations[7, 8].
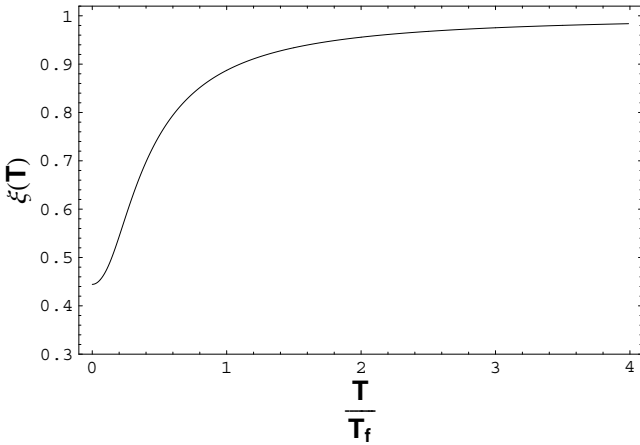

FIG. 2: The universal coefficient $\xi(T)$ versus rescaled temperature.
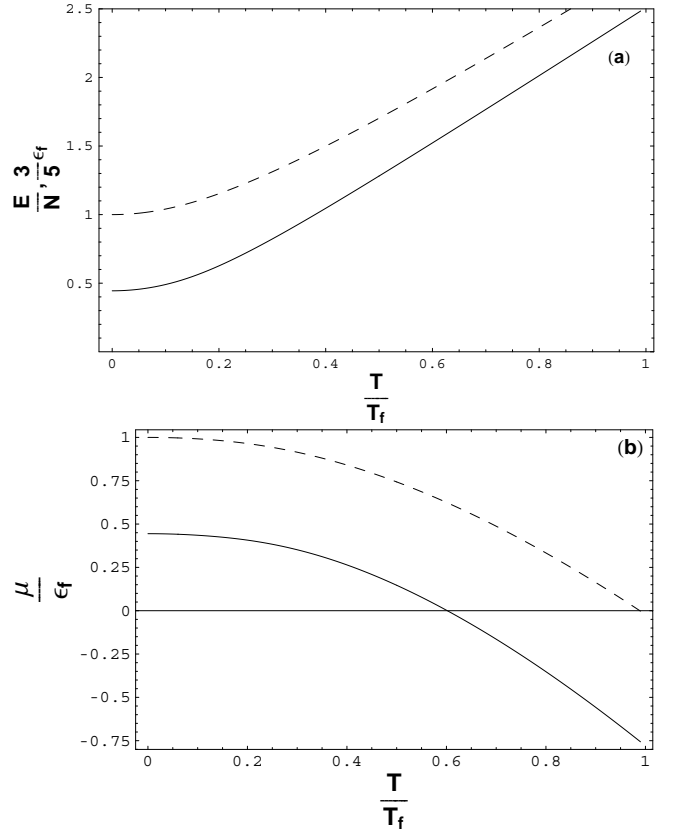

FIG. 3: a), Energy per particle versus rescaled temperature; b), the physical chemical potential. The solid curves are for the results of unitary Fermi gas. The dashed ones are those for the free Fermi gas.

C. Virial coefficients in the Boltzmann regime

To shed light on the power of the quasi-Gaussian approximation, we will consider the virial expansion for the dilute unitary Fermi system.

From the general statistical mechanics viewpoint, the virial equation of state is a series of pressure expanded in density. For the low density weak degenerate scenario $n\lambda^3 < 1$, the equation of state can be expanded according to

$$\frac{P}{nT} = \sum_{l=1}^{\infty} a_l(T)\left(\frac{n\lambda^3}{g}\right)^{l-1}. \tag{24}$$

The $a_l(T)$ is the l-order Clausius virial coefficient with g being the spin degenerate factor ($g = 2$ in this work for the ideal symmetric scenario).

For the purpose of characterizing the complex correlation effects, it is worthy noting that the expansion is according to the effective fugacity $z' = e^{\beta\mu^*}$ instead of directly according to $z = e^{\beta\mu}$. Meanwhile, in order to avoid the confusion with the conventional expansion in terms of z, the primes on b and c in the expansion identities below have been explicitly indicated. In the weak

degenerate high temperature Boltzmann regime and by using such as[29, 30]

$$f_{3/2}(z') = z' - \frac{z'^2}{2^{3/2}} + \frac{z'^3}{3^{3/2}} - \frac{z'^4}{4^{3/2}} + \cdots, \quad (25)$$

the pressure P and particle number density n are the functions of small z' and can be expanded as

$$\frac{P}{T} = \frac{2}{\lambda^3} \sum_{l=1}^{\infty} b'_l z'^l, \quad (26a)$$

$$n = \frac{2}{\lambda^3} \sum_{l=1}^{\infty} c'_l z'^l. \quad (26b)$$

By comparing Eq.(24) with Eq.(26a) and Eq.(26b), the relations between a'_l, b'_l and c'_l are derived as

$$a_1 = \frac{b'_1}{c'_1}, \quad (27a)$$

$$a_2 = b'_2 - c'_2, \quad (27b)$$

$$a_3 = b'_3 - 2b'_2 c'_2 + 2c'^2_2 - c'_3, \quad (27c)$$

$$a_4 = b'_4 - 3b'_3 c'_2 + 5b_2 c'^2_2 - 5c'^3_2 - 2b'_2 c'_3 + 5c'_2 c'_3 - c'_4, \quad (27d)$$

$$\cdots.$$

It is worthy noting that the explicit results $b'_1 = c'_1 = 1$ have been used to reduce the relations.

With the exact grand thermodynamical potential Eq.(14a) and corresponding particle number density expression Eq.(16), one can immediately obtain the dimensionless virial coefficients at unitarity $|a| = \infty$

$$a_1 = 1, \quad (28a)$$

$$a_2 = 0, \quad (28b)$$

$$a_3 = -\frac{1}{4} + \frac{4}{9\sqrt{3}} = -2a_3^{(0)}, \quad (28c)$$

$$a_4 = -\frac{15}{32} - \frac{25}{32\sqrt{2}} + \frac{5}{2\sqrt{6}} = -5a_4^{(0)}, \quad (28d)$$

$$\cdots$$

$$a_i = -\frac{(i+1)(i-2)}{2}a_i^{(0)}, \quad (28e)$$

$$\cdots.$$

The ratios of the virial coefficients for the Unitary Fermi gas to their counterparts $a_l^{(0)}$s of the ideal non-interacting Fermi gas are integers through a general term formula Eq.(28e).

D. The second virial coefficient with non-Gaussian fluctuations

From the quantum degenerate viewpoint and as in the classical van der Waals equation of state, the second virial coefficient is usually considered to be "most important". Compared with $a_2^{(0)} = \pm\frac{1}{4\sqrt{2}}$ of the ideal quantum gas with the effective quantum "attraction" $(-)$ for bosons

and "repulsion" $(+)$ for fermions, the second virial coefficient of unitary Fermi gas is found to be vanishing.

The vanishing $a_2 = 0$ is different from what was reported in the literature. In Refs.[3, 4], the simple application of the conventional quantum cluster expansion technique[29–31] gives $a_2/a_2^{(0)} \sim -3$ (note the *minus* sign). The differences between those reported in the literature and ours manifest on two respects: quantitatively, the magnitude of the second virial coefficient obtained in our approach is smaller than $a_2^{(0)}$; qualitatively, it is vanishing.

What physical reasons lead to the second virial coefficient $a_2 = 0$ with the explicit difference? In applying the perturbative quantum cluster expansion for calculating the second virial coefficient, the dilute condition $n|f_0|^3 \ll 1$ is assumed in addition to $n\lambda^3 \ll 1$. Although the divergent scattering amplitude should drop out in the final thermodynamical quantities, the dilute condition $n|f_0|^3 \ll 1$ is not automatically satisfied. In the language of resummation technique, the effects resulting from the infinite dynamical high orders with various irreducible expansion diagrams also contribute to the second virial coefficient.

In the strongly correlated medium with $n|f_0|^3 \gg 1$, especially at unitarity, the non-linear fluctuation effects and dynamical high order contribution have mutual influence. The microscopic attractive dynamics and repulsive quantum correlations are mixed with each other. Their contributions for the second virial coefficient are found to be offset at unitarity; i.e, the competitive non-linear fluctuation effects make the expected leading order quantum correction to Boyle's law vanishing.

On keeping the virial expansion up to the second order for the equation of state, the macroscopic thermodynamical property indicates an explicit Boyle tendency of a classical ideal gas. Therefore, the complicated non-Gaussian effects in the strongly correlated quantum system can be directly validated by measuring the first-order Joule-Thomson coefficient in the Boltzmann regime.

IV. PROSPECTIVE SCALING PROPERTIES AND VIRIAL EXPANSION OF UNITARY FERMI GAS

One the one hand, the essential divergence nature of the bare two-body scattering amplitude $f_0(k, a) = i/k$ implies that the weak coupling order-by-order "expansion" is not applicable with a real or virtual shallow bound state. One the other hand, the scaling property with the divergent scattering interaction strength implies that the thermodynamic expressions can be very simple; i.e., the analytical formulae or virial coefficients must be symmetrically conformal to those for the ideal noninteracting Fermi gas.

Like in the classical van der Waals equation of state, the lowest order of perturbative quantum cluster expansion in calculating a_2 is actually on the mean-field the-

ory level. In performing virial expansion at unitarity, the non-linear fluctuation effects should be reasonably well taken into account. The difficulty is reflected by the fact that the individual low and high order dynamical contributions cannot be separately described from the quantum fluctuations.

The fluctuation effects on the thermodynamics quantities beyond the mean-field theory can be described by the particle number density susceptibility. Of course, the susceptibility itself is the final goal. With this quasi-Gaussian approximation method, the integrated equation of state is uniquely determined by the particle number susceptibility χ indirectly in terms of the auxiliary variable μ^*, correlation factors $\mathcal{C}$ and $\mathcal{D}$. Through μ^*, the thermodynamical quantities can be given by a set of highly non-linear coupled equations. In the high temperature weak degenerate Boltzmann regime, the analytical virial expansion can be performed by eliminating the auxiliary variable.

As indicated by the coupled equations Eq.(14a) and Eq.(14b), the non-Gaussian fluctuation contributions compete with the high order dynamical effects. Their effects on the second virial coefficient are found to exactly cancel each other out at unitarity. Therefore, from the viewpoint of virial expansion to explore the quantum degenerate physics, one must go beyond the calculation of a_2.

A general term formula connecting the virial coefficients of ideal Fermi gas and unitary Fermi gas is found for the high order virial coefficients. With the scaling equation of state Eq.(22), the calculated virial coefficients manifest the expected scaling properties. It is worthy noting that the negative sign in front of $a_4 = -5a_4^{(0)}$ indicates a bosonization conversion tendency of the unitary Fermi gas at the *intermediate* BCS-BEC crossover point.

V. CONCLUSION

In summary, the three-dimensional strongly correlated BCS-BEC crossover thermodynamics is discussed with an auxiliary fluctuating mirror background shift method. The equations presented demonstrate a mutual influence of the quantum statistical correlation and dynamical effects for different orders.

The goal of this work is to make an analytical attempt doing the challenging non-linear virial series expansion.

The obtained results manifest the scaling property of unitary Fermi gas; i.e., the virial coefficients are found to be proportional to those of ideal Fermi gas with a general formulae.

In contrast to the investigations in the literature, the second virial coefficient of the unitary Fermi gas is found to be vanishing. To a great extent, this unpleasant result further puzzles us as regards reaching a deeper theoretical understanding of the BCS-BEC crossover physics in the Boltzmann regime.

In physics, $a_2 = 0$ would not be unexpected because the unitary Fermi system is *in between* the dimer boson and fermion phases. The non-linear fluctuation effects are mixed with and compete with the dynamical effects. Their contributions to the second virial coefficient can be exactly canceled out by each other. By keeping up to the second order virial expansion in the weakly degenerate regime, the bulk properties can manifest the Boyle's law of classical ideal gas. The Joule-Thomson Coefficient measurement in the unitary limit can clarify the difference or be used to explore the novel non-Gaussian correlation effects, in the affirmative.

In the strongly interacting regime, especially at unitarity, the non-Gaussian fluctuations play an important role. Technically, the realistic grand thermodynamical potential $\Omega(T, \mu)$ or equation of state is described by the two coupled parametric-equations Eq.(14a) and Eq.(14b). Equivalent to eliminating the implicit variable, effective chemical potential μ^*, the potential expansion is according to the effective fugacity $z' = e^{\beta\mu^*}$ instead of directly according to fugacity $z = e^{\beta\mu}$.

The virial theorem at unitarity, the general HvH theorem at zero temperature and the fundamental thermodynamical consistency relations are strictly ensured in the formulation. This non-perturbative approach makes it possible to discuss the non-Gaussian fluctuation physics in the novel strongly correlated quantum system.

[1] S. Giorgini, L.P. Pitaevskii, and S. Stringari, Rev. Mod. Phys. **80**, 1215 (2008).

[2] H. Heiselberg, Phys. Rev. **A 63**, 043606 (2001).

[3] T.-L. Ho, Phys. Rev. Lett. **92**, 090402 (2004).

[4] T.-L. Ho and E.-J. Mueller, Phys. Rev. Lett. **92**, 160404 (2004).

[5] J.E. Thomas, J. Kinast, and A. Turlapov, Phys. Rev. Lett. **95**, 120402 (2005).

[6] L. Luo, B. Clancy, J. Joseph, J. Kinast, and J. E. Thomas, Phys. Rev. Lett. **98**, 080402 (2007).

[7] A. Bulgac, J.E. Drut, and P. Magierski, Phys. Rev. Lett. **96**, 090404 (2006).

[8] E. Burovski, N. Prokof'ev, B. Svistunov, and M. Troyer, Phys. Rev. Lett. **96**, 160402 (2006); New J. Phys. **8**, 153 (2006).

[9] C.J. Horowitz and A. Schwenk, Phys. Lett. **B 638**, 153

(2006).

[10] J. Carlson, S.Y. Chang, V.R. Pandharipande, and K.E. Schmidt, Phys. Rev. Lett. **91**, 050401 (2003).

[11] A. Schwenk and C.J. Pethick, Phys. Rev. Lett. **95**, 160401 (2005).

[12] J.V. Steele, e-print arXiv:nucl-th/0010066.

[13] H.-W. Xiong, S.-J. Liu, W.-P. Zhang, and M.-S. Zhan, Phys. Rev. Lett. **95**, 120401 (2005).

[14] H. Hu, X.-J. Liu, and P.D. Drummond, Europhys. Lett.**74**, 574 (2006).

[15] G. Rupak, Phys. Rev. Lett. **98**, 090403 (2007).

[16] Y. Castin, e-print arXiv:cond-mat/0612613.

[17] J.-S. Chen, C.-M. Cheng, J.-R. Li, and Y.-P. Wang, Phys. Rev. **A 76**, 033617 (2007).

[18] G.E. Brown and M. Rho, Phys. Rep. **363**, 85 (2002).

[19] N.M. Hugenholtz and L.van Hove, Physica (Amsterdam) **24**, 363 (1958).

[20] W. Kohn and L.J. Sham, Phys. Rev. **A 140**, 1133 (1965).

[21] J.-S. Chen, Chin. Phys. Lett. **24**, 1825 (2007) and Commun. Theor. Phys. **48**, 99 (2007).

[22] L.D. Landau and E.M. Lifshitz, *Statistical Physics* (Pergamon Press, 1980).

[23] J.-S. Chen, J.-R. Li, and M. Jin, Phys. Lett. **B 608**, 39

[24] J.-S. Chen, J.-R. Li, and P.-F. Zhuang, Phys. Rev. **C 67**, 068202 (2003).

[25] J.D. Walecka, Ann. Phys. (N.Y.) **83**, 491 (1974).

[26] B.D. Serot and J.D. Walecka, Adv. Nucl. Phys. **16**, 1 (1986); Int. J. Mod. Phys. **E 6**, 515 (1997).

[27] C.J. Pethick and H. Smith, *Bose-Einstein Condensation in Dilute Gases* (Cambridge University Press, Cambridge, England, 2002).

[28] J.-S Chen, F. Qin, and Y.-P Wang, e-print arXiv:0803.4385.

[29] Kerson Huang, *Statistical Mechanics* (Wiley, New York, 1987).

[30] R.K. Pathria, *Statistical Mechanics*, (2nd edition), Butterworth-Heinemann, Oxford (1996).

[31] E. Beth and G.E. Uhlenbeck, Physica (Amsterdam) **4**, 915 (1937).

[32] G.B. Partridge, W. Li, R.I Kamar, Y.-A Liao, and R.G. Hulet, Science **311**, 503 (2006).

[33] J.T. Stewart, J.P. Gaebler, C.A. Regal, and D.S. Jin, Phys. Rev. Lett. **97**, 220406 (2006).

(2005); J.-S. Chen, e-print arXiv:nucl-th/0509038.